

# Wigner's representation of quantum mechanics in integral form and its applications

Dimitris Kakofengitis,<sup>\*</sup> Maxime Oliva,<sup>†</sup> and Ole Steuernagel<sup>‡</sup>

*School of Physics, Astronomy and Mathematics, University of Hertfordshire, Hatfield, AL10 9AB, UK*

(Dated: November 22, 2016)

We consider quantum phase space dynamics using the Wigner representation of quantum mechanics. We stress the usefulness of the integral form for the description of Wigner's phase space current  $\mathbf{J}$  as an alternative to the popular Moyal bracket. The integral form brings out the symmetries between momentum and position representations of quantum mechanics, is numerically stable, and allows us to perform some calculations using elementary integrals instead of Groenewold star-products. Our central result is an explicit, elementary proof which shows that only systems up to quadratic in their potential fulfil Liouville's theorem of volume preservation in quantum mechanics. Contrary to a recent suggestion, our proof shows that the non-Liouvillian character of quantum phase space dynamics cannot be transformed away.

PACS numbers: 03.65.-w, 03.65.Ta

## I. MOTIVATION AND INTRODUCTION

Wigner's representation of quantum mechanics in phase space [1] is equivalent to Heisenberg's, Schrödinger's and Feynman's [2]. The description of the time evolution of Wigner's phase space distribution function  $W$  uses Moyal brackets [3], the quantum analog of classical Poisson brackets. The similarity of the Moyal form with classical physics explains its popularity.

Moyal's bracket is defined as an infinite series of derivatives, which can make it cumbersome to use and also numerically unstable. It has limited applications because it assumes that the potential can be Taylor expanded. The integral form of quantum phase space dynamics [4, 5] is an alternative to Moyal's form, it also applies to piecewise or singular potentials and displays symmetries between momentum and position representation not obvious when using Moyal's formulation only.

We recently showed that in anharmonic quantum systems the violation of Liouville's volume preservation can be so large that quantum phase space volumes locally change at singular rates [6]. These singularities are of central importance, they are responsible for the generation of quantum coherences.

Here, we investigate a recent suggestion by Daligault [7]. He provided a recipe that might enable us to 'transform away' the violation of Liouville's theorem in anharmonic quantum-mechanical systems.

We illustrate the power of the integral form of Wigner's representation, it allows us to give an elementary proof that Daligault's suggestion amounts to a specific modification that makes the dynamics classical and is incompatible with his stated aim of finding a Liouvillian system that reproduces quantum dynamics.

Our proof shows that the singularities, reported in reference [6], cannot be removed to make quantum phase

space dynamics divergence-free.

## II. WIGNER'S DISTRIBUTION AND ITS EVOLUTION

In Wigner's representation of quantum mechanics [1, 8] Wigner's phase space distribution is the "*closest quantum analogue of the classical phase-space distribution*" [9], it is defined as

$$W(x, p, t) = \frac{1}{\pi\hbar} \int dy \varrho(x - y, x + y, t) e^{\frac{2i}{\hbar}py}, \quad (1)$$

$$= \frac{1}{\pi\hbar} \int ds \tilde{\varrho}(p - s, p + s, t) e^{-\frac{2i}{\hbar}xs}; \quad (2)$$

here,  $\hbar = h/(2\pi)$  is Planck's constant, integrals always run from  $-\infty$  to  $+\infty$ :  $\int = \int_{-\infty}^{\infty}$ , and  $\varrho$  and  $\tilde{\varrho}$  are the density operator in position and momentum representation, respectively.

We would like to remind the reader that out of various quantum phase space distributions [8], only Wigner's simultaneously yields the correct projections in Schrödinger's position  $\varrho(x, x, t) = \int dp W(x, p, t)$  and momentum representation  $\tilde{\varrho}(p, p, t) = \int dx W(x, p, t)$ , while maintaining its form (1) when evolved in time and giving the overlap between states in the simple form  $|\langle\psi_1|\psi_2\rangle|^2 = 2\pi\hbar \iint dx dp W_1 W_2$ . Finally, only the Wigner distribution's averages and uncertainties evolve *momentarily* classically [10, 11].

In this work we consider one-dimensional conservative systems in a pure state with quantum-mechanical Hamiltonians

$$\mathcal{H}(x, p) = \frac{p^2}{2M} + V(x). \quad (3)$$

The Wigner function's time evolution arises, in analogy to Eq. (1), from a Fourier-transform of the von Neumann

<sup>\*</sup> d.kakofengitis@herts.ac.uk

<sup>†</sup> m.oliva2@herts.ac.uk

<sup>‡</sup> O.Steuernagel@herts.ac.uk

equation  $i\hbar\frac{\partial\hat{\rho}}{\partial t} = [\mathcal{H}(\hat{x}, \hat{p}), \hat{\rho}]$  as [4, 8]

$$\begin{aligned}\partial_t W = & -\frac{p}{M}\frac{1}{\pi\hbar}\int dy \partial_x \varrho(x-y, x+y, t)e^{\frac{2i}{\hbar}py} \\ & + \frac{i}{\pi\hbar^2}\int dy [V(x+y) - V(x-y)] \\ & \times \varrho(x-y, x+y, t)e^{\frac{2i}{\hbar}py}.\end{aligned}\quad (4)$$

Throughout, we write partial derivatives as  $\frac{\partial^n}{\partial x^n} = \partial_x^n$ .

If the potential  $V$  can be globally Taylor expanded, the integral (4) yields the Moyal bracket  $\{\{\cdot, \cdot\}\}$  [3]

$$\frac{\partial W}{\partial t} = \{\{\mathcal{H}, W\}\} = \frac{1}{i\hbar}(\mathcal{H} \star W - W \star \mathcal{H}) \quad (5)$$

$$= \frac{2}{\hbar}\mathcal{H} \sin\left(\frac{\hbar}{2}\left(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right)\right)W. \quad (6)$$

Here we use Groenewold star-products  $(\star)$  [12], defined as  $f \star g = f e^{\frac{i\hbar}{2}(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)}g$ , the arrows indicate whether derivatives are executed on  $f$  or  $g$ .

Eqs. (4) or (6) can be written as the continuity equation [1]

$$\partial_t W + \nabla \cdot \mathbf{J} = \partial_t W + \partial_x J_x + \partial_p J_p = 0, \quad (7)$$

also known as the quantum Liouville equation.

Comparing Eqs. (7) and (4), we identify the Wigner current  $\mathbf{J} = (J_x)$ , with position component

$$J_x = \frac{p}{M\pi\hbar}\int dy \varrho(x-y, x+y, t)e^{\frac{2i}{\hbar}py}, \quad (8)$$

and momentum component

$$\begin{aligned}J_p = & -\frac{1}{\pi\hbar}\int dy \left[\frac{V(x+y) - V(x-y)}{2y}\right] \\ & \times \varrho(x-y, x+y, t)e^{\frac{2i}{\hbar}py}.\end{aligned}\quad (9)$$

If the potential can be Taylor-expanded, the components of Wigner current  $\mathbf{J}$  have the form [4, 13–15],

$$\mathbf{J} = \mathbf{j} + \begin{pmatrix} 0 \\ -\sum_{l=1}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \partial_p^{2l} W \partial_x^{2l+1} V \end{pmatrix}. \quad (10)$$

Here, with  $\mathbf{v} = (\frac{p}{M}, -\frac{\partial V}{\partial x})$ ,  $\mathbf{j} = W\mathbf{v}$  is the classical and  $\mathbf{J} - \mathbf{j}$  are quantum terms.

### III. FEATURES AND APPLICATIONS OF THE INTEGRAL FORM

The integral form (4) is more general than the Moyal expression since it does not rely on  $V$  being analytic.

A numerical implementation of the integral form can use Fast Fourier Transforms. In the case of potentials featuring high order Taylor terms, high order numerical derivatives can render Eq. (10) poorly convergent [15].

In reference [15] we showed (note typographical errors in Eqs. (4) and (5) of [15]) that the  $p$ -projection of  $J_x$  yields the quantum probability current  $j$  in position space

$$\begin{aligned}\int dp J_x = & \frac{\hbar}{2iM}\int dy \varrho(x-y, x+y, t)\partial_y \delta(y) \\ = & \sum_k P_k \frac{\hbar}{2iM}(\Psi_k^* \partial_x \Psi_k - \Psi_k \partial_x \Psi_k^*) = j(x, t),\end{aligned}\quad (11)$$

Here we used Dirac's- $\delta$  and wrote the density matrix as a statistical mixture of pure states

$\varrho(x, x', t) = \sum_k P_k \Psi_k(x, t) \Psi_k^*(x', t)$ . Additionally,

$$\int dx J_x = \frac{p}{M}\int ds \tilde{\varrho}(p-s, p+s, t)\delta(s) = \frac{p}{M}\tilde{\varrho}(p, p, t). \quad (12)$$

Analogously to Eq. (11), the quantum probability current  $\tilde{j}$  in momentum space [15], is

$$\begin{aligned}\int dx J_p = & -\frac{1}{\pi\hbar}\iint dy dx \left[\frac{V(x+y) - V(x-y)}{2y}\right] \\ & \times \varrho(x-y, x+y, t)e^{\frac{2i}{\hbar}py} \\ = & \frac{1}{i\sqrt{2\pi\hbar^3}}\int_{-\infty}^p dp' \int dp'' \tilde{V}^*(p'' - p')\tilde{\varrho}(p'', p') \\ & - \tilde{V}(p'' - p')\tilde{\varrho}(p', p'') = \tilde{j}(p, t),\end{aligned}\quad (13)$$

(where  $\tilde{V} = \frac{1}{\sqrt{2\pi\hbar}}\int dx V(x)e^{-\frac{i}{\hbar}px}$ ), while

$$\begin{aligned}\int dp J_p = & -\int dy \left[\frac{V(x+y) - V(x-y)}{2y}\right] \\ & \times \varrho(x-y, x+y, t)\delta(y) \\ = & -\varrho(x, x, t)\frac{dV}{dx}.\end{aligned}\quad (14)$$

We would like to emphasise that the quantum terms of Eq. (10) do not contribute in Eq. (14).

Averaging over Eqs. (12) and (14), reproduces Ehrenfest's theorem [2]

$$\int dp \frac{p}{M}\tilde{\varrho}(p, p, t) = \frac{\langle p \rangle}{M} = \frac{d\langle x \rangle}{dt} \quad (15)$$

and

$$-\int dx \varrho(x, x, t)\frac{dV}{dx} = -\left\langle \frac{dV}{dx} \right\rangle = \frac{d\langle p \rangle}{dt}. \quad (16)$$

Where applicable, the Moyal bracket formalism [2] yields the same results. Note the various subtleties associated with the interpretation of Ehrenfest's theorem [10, 11].

### IV. WHEN IS QUANTUM MECHANICAL TIME EVOLUTION LIOUVILLIAN?

To investigate whether quantum phase space dynamics is Liouvillian we determine the divergence of its quantum

phase space velocity field  $\mathbf{w}$  [7, 14, 16].  $\mathbf{w}$  is the quantum analog of the classical velocity field  $\mathbf{v}$  (Eq. (10)):

$$\mathbf{w} = \frac{\mathbf{J}}{W} = \mathbf{v} + \frac{1}{W} \left( - \sum_{l=1}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \partial_p^{2l} W \partial_x^{2l+1} V \right). \quad (17)$$

To rephrase the continuity equation (7) in terms of  $\mathbf{w}$ , we switch to the Lagrangian decomposition [7, 14, 16]

$$\frac{dW}{dt} = \partial_t W + \mathbf{w} \cdot \nabla W = -W \nabla \cdot \mathbf{w}. \quad (18)$$

Note that  $\mathbf{w}$  is singular at zeros of  $W$ , since generally zeros of  $W$  do not coincide with zeros of its derivatives. This implies, amongst other things, that the concept of trajectories in quantum phase space cannot be applied to the dynamics of anharmonic systems [6].

---

To do this, we need to establish when Wigner current obeys Liouville's theorem, when the divergence of the Wigner current's velocity field vanishes everywhere in phase space. With  $\mathbf{w} = \mathbf{J}/W$  we have

$$\nabla \cdot \mathbf{w} = \partial_x \left( \frac{J_x}{W} \right) + \partial_p \left( \frac{J_p}{W} \right) = \partial_x \left( \frac{p}{M} \right) + \partial_p \left( \frac{J_p}{W} \right) = \partial_p \left( \frac{J_p}{W} \right) = 0. \quad (19)$$

Integrating once gives us  $\int_{-\infty}^p dp' \partial_p' \frac{J_{p'}}{W} = \frac{J_p}{W} = C(x)$  which implies  $\int dp J_p = C(x) \int dp W = C(x) \varrho(x, x, t)$ . Using (9) for  $J_p$  we find that

$$\int dp J_p = - \int \left[ \frac{V(x+y) - V(x-y)}{2y} \right] \varrho(x-y, x+y, t) \delta(y) dy = -\varrho(x, x, t) \frac{\partial V}{\partial x} = C(x) \varrho(x, x, t). \quad (20)$$

It follows that  $\nabla \cdot \mathbf{w} = 0$  implies

$$J_p + \delta J_p = -W \frac{\partial}{\partial x} (V(x) + \delta V(x)). \quad (21)$$

We have shown that the application of Daligault's recipe filters through in a very specific form: the dynamics becomes classical and the shift only affects the potential (since the goal is to not affect the time evolution of  $W$ ). Strictly speaking, in Eq. (21), we should write  $\delta V(x, W(x, p, t))$  to remind ourselves of Daligault's assumption that  $\delta J_p$  depends on  $W$ . But to yield Liouvillian dynamics  $\delta V$  must not depend on  $p$ , hence  $\delta V(x, W(x, p, t)) = \delta V(x)$ .

For systems in which the potential can be globally Taylor-expanded, Eq. (21) shows us that quantum terms must not be present in Eq. (10). To fulfil Liouvillian behaviour for all times the potential  $V$  might be of 'harmonic' form:  $V = V_{\text{harmonic}} = \frac{K}{2}x^2 + ax + b$  with arbitrary real  $K$ ,  $a$  and  $b$ , and therefore  $\delta V = 0$ .

Alternatively, the auxiliary field has the trivial form  $\delta \mathbf{J} = \mathbf{j} - \mathbf{J}$  which subtracts all the quantum parts in Eq. (10), so that the potential assumes the form  $V + \delta V = V_{\text{harmonic}}$ . This is neither what Daligault intended nor is it helpful, in fact, it is not even permissible since such a field would not fulfil the condition  $\nabla \cdot \delta \mathbf{J} = 0$ .

Problems associated with the singularities have been observed multiple times [16, 17], they badly affect numerical quantum phase space studies [16].

It would therefore be intriguing to be able to transform such problems away, as has been suggested by Daligault [7]. He speculated that it might be possible to add an auxiliary field  $\delta \mathbf{J}$  to  $\mathbf{J}$  in Eq. (7) which would not modify the dynamics since it is assumed to be divergence-free. Yet, this auxiliary field might yield a modification to the velocity field such that their sum fulfils Liouville's theorem:  $\nabla \cdot (\mathbf{w} + \delta \mathbf{w}) = 0$ . If possible, we could deploy the machinery of classical phase space transport equations to solve quantum problems.

We now prove that we cannot get rid of the non-Liouvillian character of quantum phase space dynamics in anharmonic systems in the way Daligault suggested.

---

One might wonder whether there is some other option, perhaps the anharmonic quantum terms  $\mathbf{J} - \mathbf{j}$  in Eq. (10) are present but the initial state  $W_0$  has some special form that cancels all anharmonic terms yet does not force the trivial form  $V + \delta V = V_{\text{harmonic}}$  on us.

This cannot be though: if  $J_p + \delta J_p$  fulfils Eq. (21), the dynamics is classical and anharmonic, shearing the phase space distribution. Since a Wigner distribution can be expanded in the coherent state basis, we assume, without loss of generality, that the initial state  $W_0$  is a coherent state. Classically shearing a phase space distribution bends it out of shape while keeping it positive, this violates the constraint that a positive Wigner distribution has Gaussian form [18]: anharmonic positivity-preserving classical dynamics is incompatible with quantum phase space dynamics.

Generalising Daligault's recipe slightly: might modifications to the  $J_x$  component help? We doubt it, if the system is Hamiltonian, even if not quantum-mechanical but, say, of the classical Kerr-oscillator type, one would, according to Eq. (18), still end up with Liouvillian dynamics:  $\frac{d}{dt} W = 0$ .  $W$  cannot change sign, Daligault's recipe could never give us quantum dynamics, i.e., negativity formation in phase space [6].

Mappings of the phase space dynamics of an anhar-

monic quantum-mechanical system onto the dynamics of a classical dynamical system that fulfils Liouville's theorem and features the same time evolution do not exist.

In their monograph on the Wigner representation, Zachos *et al.* [2] argue that anharmonic quantum systems cannot fulfil Liouville's theorem since the difference between the Moyal and Poisson brackets are non-zero for anharmonic quantum systems. In light of Daligault's speculation that a mapping to *another* system might exist, that reproduces the same dynamics and fulfils Liouville's theorem, we feel the above proof with the explicit

use of  $\mathbf{J}$  is needed to settle the matter.

## V. CONCLUSION

We showed that the integral form of Wigner's representation of quantum mechanics should be consulted as an alternative to Moyal's formulation. It is more general than Moyal's form. If high order derivatives are present in Moyal's form, the integral form tends to converge better in numerical calculations. It can make mathematical manipulations more transparent than Moyal's form, and it displays symmetries between position and momentum configuration space more clearly.

- 
- [1] E. Wigner, *Phys. Rev.* **40**, 749 (1932).
  - [2] C. K. Zachos, D. B. Fairlie, and T. L. Curtright, *World Scientific* **34** (2005), 10.1142/5287.
  - [3] J. E. Moyal, *Proc. Camb. Phil. Soc.* **45**, 99 (1949).
  - [4] E. Wigner, *Phys. Rev.* **40**, 749 (1932).
  - [5] G. A. Baker, *Phys. Rev.* **109**, 2198 (1958).
  - [6] M. Oliva, D. Kakofengitis, and O. Steuernagel, *ArXiv e-prints* (2016), arXiv:1611.03303 [quant-ph].
  - [7] J. Daligault, *Phys. Rev. A* **68**, 010501 (2003).
  - [8] M. Hillery, R. F. O'Connell, M. O. Scully, and E. P. Wigner, *Phys. Rep.* **106**, 121 (1984).
  - [9] W. H. Zurek, *Nature* **412**, 712 (2001), quant-ph/0201118.
  - [10] A. Royer, *Found. Phys.* **22**, 727 (1992).
  - [11] L. Ballentine, Y. Yang, and J. Zibin, *Physical review A* **50**, 2854 (1994).
  - [12] H. J. Groenewold, *Physica* **12**, 405 (1946).
  - [13] R. T. Skodje, H. W. Rohrs, and J. Vanbuskirk, *Phys. Rev. A* **40**, 2894 (1989).
  - [14] A. Donoso and C. C. Martens, *Phys. Rev. Lett.* **87**, 223202 (2001).
  - [15] O. Steuernagel, D. Kakofengitis, and G. Ritter, *Phys. Rev. Lett.* **110**, 030401 (2013), 1208.2970.
  - [16] C. J. Trahan and R. E. Wyatt, *J. Chem. Phys.* **119**, 7017 (2003).
  - [17] R. Sala, S. Brouard, and J. G. Muga, *J. Chem. Phys.* **99**, 2708 (1993).
  - [18] R. Hudson, *Rep. Math. Phys.* **6**, 249 (1974).